

Required parameters for each module. The QSP-IO identifier is to be used for the `name` field in the JSON parameter file verbatim.

Module	Parameter	Variable Name	QSP-IO Identifier
All	central compartment volume	V_C	<code>V_C</code>
	peripheral compartment volume	V_P	<code>V_P</code>
	cancer-free tumor compartment volume	$V_{T\min}$	<code>V_Tmin</code>
	lymph node compartment Volume	V_{LN}	<code>V_LN</code>
	cancer cell volume	V_{cancer}	<code>vol_cell</code>
	T cell volume	V_{Tcell}	<code>vol_Tcell</code>
Cancer	dead cell clearance rate	k_{clear}	<code>k_cell_clear</code>
	rate of cancer cell growth	k_{growth}	<code>k_C_growth</code>
	cancer cell capacity	C_{max}	<code>C_max</code>
	rate of cancer cell death	k_{inact}	<code>k_C_death</code>
T Cell	initial tumor diameter	$D_T(0)$	<code>initial_tumour_diameter</code>
	T cell receptor diversity	—	<code>div</code>
	T cell clonality	n_{clones}	<code>n_clones</code>
	thymic output of naïve T cells ¹	σ	<code>Q_nT_thym</code>
	rate of T cell transport into P	q_P^{in}	<code>q_P_in</code>
	rate of T cell transport out of P	q_P^{out}	<code>q_P_out</code>
	rate of T cell transport into T	q_T^{in}	<code>q_T_in</code>
	rate of T cell transport into LN	q_{LN}^{in}	<code>q_LN_in</code>
	rate of T cell transport out of LN	q_{LN}^{out}	<code>q_LN_out</code>
	naïve T cell count in C	$\mathcal{N}_C(0)$	<code>nT_C</code>
	naïve T cell count in P	$\mathcal{N}_P(0)$	<code>nT_P</code>
	naïve T cell count in LN	$\mathcal{N}_{LN}(0)$	<code>nT_LN</code>
	rate of naïve T cell death	k_{death}^N	<code>k_nT_death</code>
	rate of T cell activation	k_{act}	<code>k_act</code>
	rate of naïve T cell proliferation ¹	k_{prolif}	<code>k_nT_pro</code>
T Cell	K_m for naïve T cell proliferation ¹	K_m	<code>K_nT_pro</code>
	rate of T cell proliferation	k_{pro}	<code>k_pro</code>
	rate of T cell death	k_{death}^T	<code>k_death</code>
	rate of cancer death by T cells	k_{Tcell}	<code>k_C_Tcell</code>
	rate of T cell exhaustion by cancer	k_C	<code>k_Tcell</code>
	rate of IL2 degradation	k_{deg}^{IL2}	<code>k_IL2_deg</code>
	rate of IL2 secretion	k_{sec}	<code>k_IL2_sec</code>
	rate of IL2 consumption	k_{cons}	<code>k_IL2_cons</code>
	K_m for IL2 consumption	$[IL2]_{50}$	<code>IL2_50</code>
	K_m for IL2 consumption by Tregs	$[IL2]_{50}^{Treg}$	<code>IL2_50_Treg</code>

	baseline mean division destiny	N_0	NO
	division destiny increase from IL2	ΔN	N_{IL2}
Treg	Treg receptor diversity	—	div_Treg
	Treg clonality	n_{clones}	$n_{\text{clones_Treg}}$
	rate of T cell exhaustion from Tregs	k_{Treg}	k_{Treg}
	thymic output of naïve Tregs ¹	σ	$Q_{\text{nT_thym_Treg}}$
	rate of Treg transport into P	q_{P}^{in}	$q_{\text{P_in_Treg}}$
	rate of Treg transport out of P	$q_{\text{P}}^{\text{out}}$	$q_{\text{P_out_Treg}}$
	rate of Treg transport into T	q_{T}^{in}	$q_{\text{T_in_Treg}}$
	naïve Treg count in C	$\mathcal{N}_{\text{C}}(0)$	$n_{\text{Treg_C}}$
	naïve Treg count in P	$\mathcal{N}_{\text{P}}(0)$	$n_{\text{Treg_P}}$
	naïve Treg count in LN	$\mathcal{N}_{\text{LN}}(0)$	$n_{\text{Treg_LN}}$
	rate of Treg activation	k_{act}	$k_{\text{act_Treg}}$
	rate of naïve Treg proliferation ¹	k_{prolif}	$k_{\text{nT_pro_Treg}}$
	rate of Treg proliferation	k_{pro}	$k_{\text{pro_Treg}}$
	rate of Treg death	k_{death}^T	$k_{\text{death_Treg}}$
APC	rate of APC maturation	k_{mat}	$k_{\text{APC_mat}}$
	rate of APC migration	k_{mig}	$k_{\text{APC_mig}}$
	rate of APC death	k_D	$k_{\text{APC_death}}$
	rate of mature APC death	$k_{\hat{D}}$	$k_{\text{mAPC_death}}$
	steady-state APC count in T	ρ_{T}^D	APCO_T
	steady-state APC count in LN	ρ_{LN}^D	APCO_LN
	cytokine rate constant	k_c	k_c
	baseline cytokine concentration	$[c]_0$	c_0
	K_m for cytokine maturation	$[c]_{50}$	c_{50}
	concentration of cytokines released by cancer death	x_c	DAMPs
Antigen	number of T cell-APC binding sites	n_{sites}	$n_{\text{sites_APC}}$
	number of MHC molecule types	—	N_{MHC}
	total number of MHC moledule per unit area	$[M]_{\text{total}}$	MHC_T
	rate of MHC internalization	k_{in}	k_{in}
	rate of MHC externalization	k_{out}	k_{out}
	endosomal volume	V_e	V_e
	endosomal surface area	A_e	A_e
	APC surface area	A_s	A_s
	rate of antigen uptake	k_{up}	k_{up}
	rate of extracellular antigen degradation	k_{deg}	$k_{\text{xP_deg}}$
	rate of endosomal antigen degradation	k_{deg}^P	$k_{\text{P_deg}}$
	rate of endosomal epitope degradation	k_{deg}^P	$k_{\text{p_deg}}$

	antigen association constant	k_{on}	k_on
	APC-T cell synapse surface area	A_{syn}	A_syn
	cancer cell surface area	A_C	A_cell
	T cell surface area	A_{Tcell}	A_Tcell
	rate of TCR modification	k_p	k_TCR_p
	rate of TCR binding	$k_{\text{on}}^{\text{TCR}}$	k_TCR_on
	rate of TCR unbinding	$k_{\text{off}}^{\text{TCR}}$	k_TCR_off
	rate of TCR modification leading to non-signaling	ϕ	phi_TCR
	number of intermediate states in KPR model	m	N_TCR
	number TCR molecules per unit area	TCR_{tot}	TCR_tot
	K_m for antigen presentation signal	$K_{p,50}$	p_50
PD1	APC surface area	A_s	A_s
	APC-T cell synapse surface area	A_{syn}	A_syn
	cancer cell surface area	A_C	A_cell
	T cell surface area	A_{Tcell}	A_Tcell
	PD1 expression on T cells	—	T_PD1_total
	PDL1 expression on cancer cells	—	C_PDL1_total
	PDL2 expression on cancer cells	—	C_PDL2_total
	PDL1 expression on APCs	—	APC_PDL1_total
	PDL2 expression on APCs	—	APC_PDL2_total
	PD1/PDL1 binding rate	$k_{\text{on}}^{YY_1}$	k_on_PD1_PDL1
	PD1/PDL1 unbinding rate	$k_{\text{off}}^{YY_1}$	k_off_PD1_PDL1
	PD1/PDL2 binding rate	$k_{\text{on}}^{YY_2}$	k_on_PD1_PDL2
	PD1/PDL2 unbinding rate	$k_{\text{off}}^{YY_2}$	k_off_PD1_PDL2
	PD1/anti-PD1 binding rate	k_{on}^{YA}	k_on_PD1_aPD1
	PD1/anti-PD1 unbinding rate	k_{off}^{YA}	k_off_PD1_aPD1
	PDL1/anti-PDL1 binding rate	$k_{\text{on}}^{Y_1 A_1}$	k_on_PDL1_aPDL1
	PDL1/anti-PDL1 unbinding rate	$k_{\text{off}}^{Y_1 A_1}$	k_off_PDL1_aPDL1
	anti-PD1 cross-binding efficiency	χ	Chi_PD1
	anti-PDL1 cross-binding efficiency	χ_1	Chi_PDL1
	K_m for PD1/PDL1 checkpoint inhibition	$PD1_{50}$	PD1_50
	Hill coefficient for PD1/PDL1 checkpoint inhibition	n	nPD1

¹These parameters are normalized by T cell receptor diversity in QSP-IO, e.g., $\sigma = Q_n T_{\text{thym}} / \text{div}$